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STRONG *LSJ* DEPENDENCE OF FLUORESCENCE YIELDS: BREAKDOWN OF THE CONFIGURATION-AVERAGE APPROXIMATION

M. F. HASOĞLU, T. W. GORCZYCA, AND K. T. KORISTA
Department of Physics, Western Michigan University, Kalamazoo, MI 49008-5252; gorczyca@wmich.edu
S. T. MANSON
Department of Physics and Astronomy, Georgia State University, Atlanta, GA 30303
N. R. BADNELL
Department of Physics, University of Strathclyde, Glasgow G4 0NG, UK
AND
D. W. SAVIN
Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027
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ABSTRACT

Using the five-electron K-shell vacancy $1s2s^22p^2$ configuration as an example, we show that the fluorescence yields of the eight *LSJ* states of the configuration exhibit a dramatic dependence on *LSJ*. These results demonstrate that, in general, configuration-average fluorescence data are inappropriate for astrophysical modeling.

Subject headings: atomic data — atomic processes — line: formation — X-rays: general

1. INTRODUCTION

The advent of the new satellites making astronomical observations in the X-ray range with unprecedented precision and resolution, e.g., *Chandra* and *XMM-Newton*, has engendered a need for inner-shell atomic and ionic data to interpret these observations. Unlike outer shells of atoms and ions, where the removal of an electron results in only limited relaxation and (generally) no further transitions, inner-shell ionization *always* leads to very significant relaxation and is *always* followed by subsequent radiative and/or Auger transitions filling the inner-shell vacancy (Crasemann 1975, 1985).

Among the most important data for astrophysical modeling concerning inner-shell vacancies is the fluorescence yield, the probability that the vacancy will decay radiatively, because the emission of X-rays as opposed to Auger electrons has differing effects on an astrophysical plasma. Highly accurate calculated values are required to apply to the new astronomical observations. The most widely used extant fluorescence yield database (Kaastra & Mewe 1993) is based on configuration-average atomic theory, and these data are used in various astrophysical modeling codes, e.g., CLOUDY (Ferland et al. 1998), XSTAR (Kallman & Bautista 2001), and the SNR code of Borkowski et al. (2001). Gorczyca et al. (2003, 2006) showed that the configuration-average fluorescence yields given by Kaastra & Mewe (1993) are inaccurate, owing to the simple approximations and extrapolations made. In this communication, it is shown that the configuration-average fluorescence yield is inapplicable in astrophysical situations.

To illustrate these points, fluorescence yields of the astrophysically important five-electron boron-like core-excited $1s2s^22p^2$ isoelectronic sequence are considered. Results of our state-of-the-art calculations for the sequence are presented. These calculations are carried out for each member of the sequence from singly ionized C^+ to 25 times ionized Zn^{25+}, and they reveal a dramatic dependence of the fluorescence yields on the specific *LSJ* state of the atomic $1s2s^22p^2$ configuration.

2. THEORETICAL METHODOLOGY

Inner-shell vacancy states decay either by fluorescence, with radiative rate A_r, or by electron emission, with autoionization rate A_a. For our particular case, the possible pathways are

$$1s2s^22p^2(^{2S+1}L_J) \overset{A_{r1}}{\rightarrow} 1s^22s^22p(^2P^o_{J'}) + h\nu. \quad (1)$$

$$\overset{A_{r2}}{\rightarrow} 1s^22p^3([^4S, {}^2D, {}^2P]_{J'}) + h\nu. \quad (2)$$

$$\overset{A_{a1}}{\rightarrow} 1s^22s^2(^1S_0) + e^-. \quad (3)$$

$$\overset{A_{a2}}{\rightarrow} 1s^22s2p(^{1,3}P^o_{J''}) + e^-. \quad (4)$$

$$\overset{A_{a3}}{\rightarrow} 1s^22p^2([^1S, {}^3P, {}^1D]_{J'''}) + e^-. \quad (5)$$

We note here that, at the single-particle level of description, the radiative rate A_{r1} in equation (1) equals zero for the initial ^4P_J states due to spin conservation, and the radiative rate A_{r2} in equation (2) equals zero for all *LSJ* initial states as this is a two-electron transition. In addition, the partial Auger rate A_{a1} in equation (3) equals zero for the initial $^{2,4}P_J$ states due to parity conservation.

The K-shell fluorescence yield, the probability for radiative decay versus Auger decay, is given by

$$\omega_K \equiv \frac{A_r}{A_r + A_a}. \quad (6)$$

We employ the atomic structure and collision code AUTOSTRUCTURE (Badnell 1986) to calculate ab initio matrix elements contributing to the various energy levels and rates A_r and A_a. In these multiconfiguration Breit-Pauli (MCBP) calculations, the most important configuration interaction (CI)—the $2s^2 \rightarrow 2p^2$ intrashell correlation—is included as well as semirelativistic effects such as the spin-orbit interaction. In-

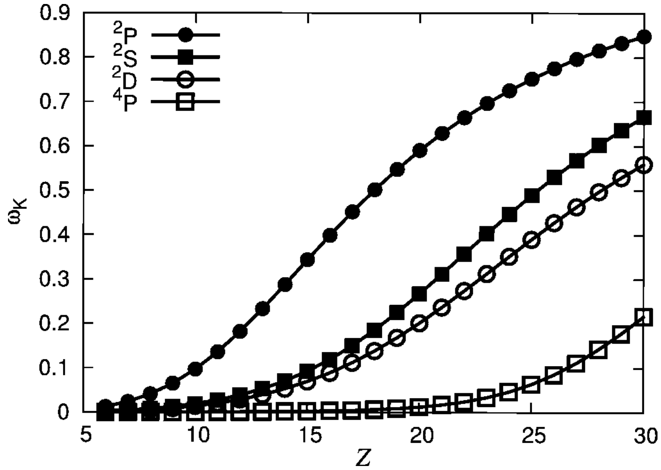

FIG. 1.—Calculated fluorescence yields ω_K for K-shell vacancy boron-like $1s2s^22p^2(^{2S+1}L)$ statistically averaged over their respective J-levels showing the LS dependence.

cluding this correlation goes beyond the single-particle model used by Kaastra & Mewe (1993). These effects become increasingly important as the nuclear charge Z increases. Certain decay pathways forbidden in equation (1) are nonnegligible once CI and semirelativistic effects are considered. For instance, the initial ^4P_J states cannot radiate at the single-particle level. However, by considering mixing the $1s2s^22p^2(^4P_J)$ configuration with the $1s2p^4(^4P_J)$ configuration, via the intrashell correlation, and with the $1s2s^22p^2(^2L_J)$ configurations, via the spin-orbit interaction, radiative decay is no longer forbidden and indeed eventually dominates at higher Z. Note also that our present AUTOSTRUCTURE calculations were performed with nonorthogonal sets of orbitals optimized separately on the initial and final states, thereby allowing for the strong relaxation effects between single- and double-K-shell vacancy states. For the work here, all the individual rates are calculated for each of the possible LSJ states. The calculations include every member of the isoelectronic sequence up to boron-like Zn^{25+}.

3. RESULTS AND DISCUSSION

To begin with, the five-electron K-shell vacancy $1s2s^22p^2$ configuration can be in one of four LS states: $^{2,4}P$, ^2S, and ^2D. Furthermore, ^2P can be in the $J = 1/2$ or $3/2$ states, ^2D in 3/2 or 5/2 states, ^4P in 1/2, 3/2, or 5/2 states, and ^2S in the 1/2 state. In other words, the $1s2s^22p^2$ configuration can be in any of *eight LSJ* states. The K-shell fluorescence yields of each of these eight states have been calculated, as described above. In order to focus on the various effects individually, the results for the four LS states (statistically averaged over the various J-components) are shown for the entire isoelectronic sequence in Figure 1. The outstanding feature of these results is the dramatic difference among the K-shell fluorescence yields corresponding to the various LS states of the $1s2s^22p^2$ configuration. For example, at $Z = 20$, the lowest fluorescence yield is close to zero, while the largest is seen to be about 0.6. Considering that the fluorescence yield can only vary between 0 and 1, this amounts to an extremely large difference. In any case, owing to the large differences in fluorescence yield among the various LS states arising from the $1s2s^22p^2$ configuration, there can be no single fluorescence yield that approximates them all.

But this is only part of the story. The fluorescence yields for the various J-states for each of the LS multiplets are shown in Figure 2 for ^4P, ^2P, and ^2D where significant variations of the fluorescence yield among the J-components of a given LS multiplet are also evident. At $Z = 30$, the lowest fluorescence yield is about 0.1, and the highest is roughly 0.9. This further hammers home the point that using configuration-averaging to generate an approximate single fluorescence yield for all LSJ states of a given configuration can be quite wrong. Implicit in this conclusion is that each of the various radiative and Auger decay rates, on which the fluorescence yields depend, are also state-dependent and cannot be approximated well by average rates for the configuration.

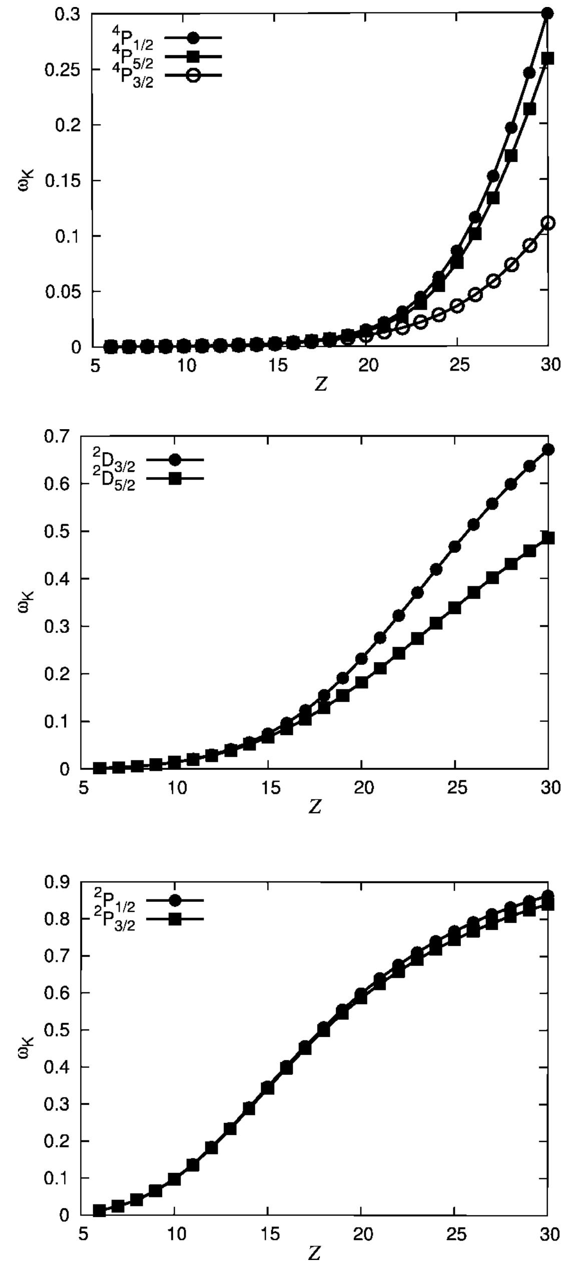

FIG. 2.—Calculated fluorescence yields ω_K for K-shell vacancy boron-like $1s2s^22p^2(^{2S+1}L_J)$ showing the LSJ dependence.

Before proceeding further, it is of some importance to look at the accuracy of our present MCBP results. Fortunately, there are calculations of Chen & Crasemann (1987) that treat some members of the five-electron isoelectronic sequence based on a fully relativistic, multiconfiguration Dirac-Fock (MCDF) method. A comparison over the isoelectronic sequence for the

$1s2s^22p^2(^2D_{3/2})$ initial state is shown in Figure 3. Agreement of the present work with the Chen & Crasemann (1987) results are excellent, indicating both that the important many-body effects are included and that the Breit-Pauli approach takes into account all of the important relativistic effects. Since the Chen & Crasemann (1987) calculations are only for selected ions in the isoelectronic sequence, and completeness is a required attribute of atomic data for astrophysics, new calculations were needed.

The *LSJ* dependence of the fluorescence yields is the result of a number of factors. The ^4P states are qualitatively different from the other multiplets in that at the single-particle level, they are forbidden to radiate so that their fluorescence yields would be zero. A nonzero radiation rate, and thereby a nonzero fluorescence yield, is engendered by CI and spin-orbit mixing. Owing to CI, $1s2s^22p^2(^4P)$ acquires a $1s2p^4(^4P)$ component that *can* radiate down to $1s2s2p^3(^4S)$ and $1s^22p^3(^4S)$. More importantly, the spin-orbit interaction mixes the ^4P_J state with the doublet states of the same J. Thus, the $^4P_{5/2}$ state mixes with $^2D_{5/2}$, $^4P_{3/2}$ mixes with $^2D_{3/2}$ and $^2P_{3/2}$, and $^4P_{1/2}$ mixes with $^2P_{1/2}$ and $^2S_{1/2}$. This differential mixing results in differing radiative and Auger decay rates that translates to the different fluorescence yields among the ^4P_J states.

For the doublet states, the situation is different because the decays are basically single-particle processes modified only somewhat by CI. In these cases, the differing decay rates (and, therefore, fluorescence yields) are simply the result of parity and angular momentum conservation, along with the differing angular momentum geometry of the transitions in the various decay channels, both radiative and Auger, that depend strongly on *LSJ* of the initial K-shell vacancy state. As an example, the ^2D and ^2S states can undergo Auger transitions to the ground $1s^22s^2(^1S)$ state *and* the excited $1s^22s2p(^{1,3}P)$ and $1s^22p^2(^1S, ^3P, ^3D)$ states of the four-electron ion, but ^2P is parity-forbidden from decaying to the four-electron ground state *via* the Auger process. We note parenthetically that ^4P can Auger-decay *only* to the excited four-electron states.

Furthermore, in order to use any kind of *average* fluorescence yield in modeling an astrophysical plasma, it is necessary to know the relative populations of each of the *LSJ* states since the individual fluorescence yields are so different. It is, nevertheless, possible to define an average fluorescence yield for a configuration as

$$\omega_K^{av} = \sum_{LSJ} a_{LSJ}\,\omega_K^{LSJ}, \qquad (7)$$

where the ω_K^{LSJ} are the state-specific K-shell fluorescence yields and the a_{LSJ} represent the number of ions in the given *LSJ* state as a fraction of the total number of ions in the configuration. But the relative populations of the *LSJ* states, the a_{LSJ}, are clearly a function of the particular astrophysical situation and will be very different for different plasma conditions. For example, if the five-electron $1s2s^22p^2$ configuration is produced *via* photoionization or electron impact ionization of the six-electron $1s^22s^22p^2$ ion in its ground ^3P state, the ^2P and ^4P states of the five-electron system will be produced in nonnegligible quantities, owing to angular momentum selection rules. In addition, if the five-electron $1s2s^22p^2$ configuration is produced *via* dielectronic recombination with the ground ^1S state of the four-electron system $1s^22s^2$, the quartet states of the five-electron ion will be produced with much lower probability than the doublets since quartet production requires a spin-flip transition. Other scenarios can be envisioned as well, each producing its own unique relative populations of the *LSJ* states of the five-electron ion. Evidently then, the notion of an average fluorescence yield for the $1s2s^22p^2$ configuration is not a useful one for astrophysical modeling.

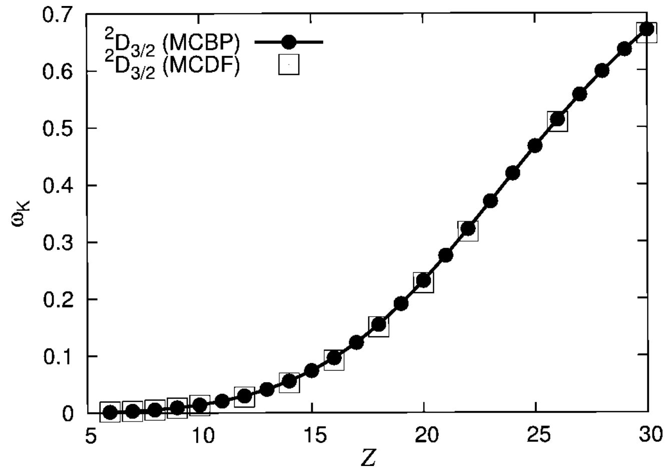

FIG. 3.—Calculated fluorescence yields ω_K for K-shell vacancy boron-like $1s2s^22p^2(^2D_{3/2})$ comparing the present MCBP results to the MCDF results of Chen & Crasemann (1987).

4. CONCLUSIONS

In this communication, it has been shown that the fluorescence yields of the eight *LSJ* states arising from the five-electron K-shell vacancy $1s2s^22p^2$ configuration are strongly *LSJ*-dependent over the entire isoelectronic series. This finding implicitly shows that the individual transition rates, radiative and Auger, are also strongly *LSJ*-dependent. In addition, the fundamental reasons for this dependence have been indicated. But there is nothing special about the five-electron K-shell vacancy system; the same general phenomenology should be true for other isoelectronic sequences with fewer than 10 electrons as well (i.e., the conclusions for the system considered should be quite general).[1] For use in astrophysical modeling codes, then, fluorescence yields, and the radiative and Auger rates associated with them, need to be given for individual *LSJ* states; the oft-used Kaastra & Mewe (1993) data compilation contains configuration-average fluorescence yields, and these are quite inappropriate for most astrophysical situations. In other words, if configuration averages are sought, they cannot be general but must be tailored to the specific astrophysical situation being considered.

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[1] For systems with 10 or more electrons, Palmeri et al. (2003) and Mendoza et al. (2004) have demonstrated in the case of iron ions that the fluorescence yields become almost independent of the *LSJ* state of the outermost shells because the intermediate-shell radiative and Auger decay transitions to the K shell are dominant.

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